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Interplay of fluid rheology and flow actuation for modulation of mixing characteristics in T-shaped microchannels

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Abstract. Microfluidic applications demand mixing of fluids in a small span of length and time, which remains a challenging task due to the low Reynolds number flows at these scales. The mixing analysis becomes further complex with non-Newtonian fluids, which often have high effective viscosity. Such fluids are frequently encountered in practical applications. In the present study, we numerically analyze an effective way of mixing time-independent inelastic liquids using pulsatile velocity inlet conditions using COMSOL Multiphysics. The fluids are considered to obey the power law model for the rheological analysis. We demonstrate enhanced mixing using pulsing velocity inlet condition and achieve superior values of mixing by tuning the interplay of pulsed input velocity and phase difference between the input pulses. The analysis is done for both shear-thinning and shear-thickening fluids, and enhanced mixing is demonstrated. It was observed that upon pulsing, a mixing of 86%, 84.4% and 82.9% for n = 0.6, n = 1, and n = 1.4 respectively occurred. It was also observed that by introducing a phase difference of 180°, the mixing index increased by 13.2%, 5.8% and 3.9% for n = 0.6, n = 1, and n = 1.4 respectively. Maximum mixing of 97.6% was observed for shear thinning liquid (n = 0.6) at a pulsatile input conditions having a phase difference of 180°. It was also observed that upon increasing the frequency of pulsation, the mixing decreases. This study will be helpful in designing micromixers for the effective mixing of non-Newtonian liquids in a small span of length and time.

Keywords. Micromixer; pulsatile flow; non-Newtonian fluids; power law; mixing index.

1. Introduction

Microfluidics is an interdisciplinary research domain that deals with fluid flow in micro confinements. Owing to the advantages like excellent operating stability and enhanced transport properties [1], microfluidic devices have been used in various applications ranging from molecular diagnostics [2] to electronic cooling [3, 4], power generation [5], and micro-mixing [6, 7]. The mixing of two chemical reagents is a critical issue in any procedure, regardless of the application. However, it remains a challenge in microchannels owing to the laminar nature of the flow. To improve mixing, many researchers have implemented various techniques which can be broadly classified as active and passive techniques. Active techniques implement external energy like [8], magnetic and electric fields [8, 9], and acoustics [10], while passive techniques implement geometric modifications [11, 12]. One of the effective techniques is time-dependent inlet velocity condition [2, 13, 14] owing to its simplicity in practical applications. The most intuitive way of increasing mixing in microchannels is by introducing obstructions in the channel, which generate vortices to enhance mixing. This has been studied extensively by many researchers [15–20]. However, the fabrication of these special geometries in micro-domains becomes complicated due to their smaller size and required accuracy and precision. As a result of this, a relatively simpler method of pulsed velocity inlet has attracted the attention of many researchers [2, 14, 21, 22].

Mixing enhancement was reported for Newtonian fluid by Glasgow and Aubry [2]. They studied the effect of various combinations of pulsing and non-pulsing sinusoidal inlet velocity conditions on the mixing of liquids with

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different concentrations of dye, thereby making it easier to visualize mixing. The mixing time was observed to reduce drastically as compared to the constant velocity inlet, and it was observed that the optimal mixing condition occurs when the phase angle between two pulsed inputs is 180°. The effect of different microchannel geometry on mixing under pulsed inlet conditions show that the effect of pulsing results in better mixing than that obtained by geometric variations in the microchannel. The combination of geometric variation with pulsed input results in a substantial increase in the mixing of two fluids [21]. Similarly, Afzal and Kim [14] have implemented pulsed flow with geometric modifications and reported an increase of 19% in the mixing index. These analyses have been done with Newtonian fluids.

The majority of microfluidic devices utilized in medical applications, such as micromixers, deal with fluids that are non-Newtonian. Thus, it is necessary to appreciate the mixing of such fluids in the micro-domain. In this study, simulations are performed to analyze the mixing behavior of non-Newtonian fluid under the influence of time-varying input conditions. Tatlısoz and Canpolat [22] have studied the mixing of Newtonian and non-Newtonian fluid under the action of pulsatile input and electric field in a straight microchannel with rectangular obstruction and reported an increase of 60% in the mixing index of non-Newtonian fluid.

From the literature reviewed, it is observed that a significant amount of work has been done in analyzing the mixing characteristics of Newtonian fluids by the use of both geometric variations and pulsed velocity inlets. Studies on the combined effects of pulsed inlet velocity, obstructions, and electric field on the mixing of non-Newtonian fluids in microchannels having inlets on the same plane have also been reported [22]. However, the study of the mixing of non-Newtonian fluids in microchannels with perpendicular inlets and pulsed input has not been reported to the best of the author's knowledge.

In the present study, we numerically investigate the effect of pulsatile inlet velocity conditions on the mixing of non-Newtonian fluids in a T shape microchannel with inlets perpendicular to each other. We chose this configuration as it is widely used in applications like macromolecule characterization like DNA, RNA, proteins [23], for diagnosis-based lab-on-a-chip devices [24], particle separation and analysis [25], and droplet generation [26]. We study the effect of pulsed inlet condition, pulsing frequency, and phase difference on the mixing index and report the optimum frequency and phase difference required to obtain the maximum mixing index. In this work, we have not included any other active fields that would help set a benchmark case for further development of micromixers with such configurations.

2. Materials and methods

2.1 *Geometry*

Figure 1 shows a schematic of a T-shaped channel which has a rectangular cross-section and perpendicular inlets. The inlet arms for fluids A and B are considered of length 1.25 mm, each and the channel spans over a distance of 3 mm after the confluence. The channel has width and height of 200 μm and 120 μm, respectively.

2.2 *Numerical modelling*

We perform a 3-D numerical study and solve the governing equations for modelling the physics involved. The equations are as follows-

Continuity equation

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

Momentum equation

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = \nabla\cdot\left[-p\mathbf{I} + \left\{\mu_{app}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)\right\}\right] \tag{2}$$

Where, $\mathbf{u}$ is the velocity vector, ρ is the density of the liquid, $\mathbf{I}$ is the identity matrix, p denotes pressure, and μ_{app}

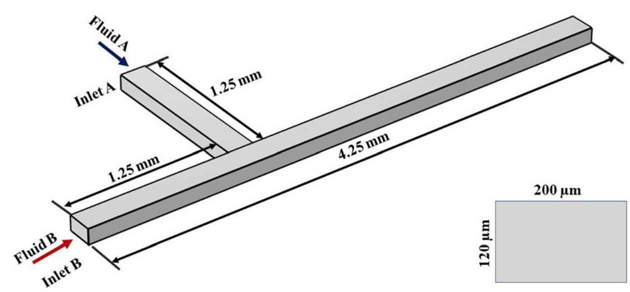

Figure 1. Schematic of analysis domain.

Table 1. Mesh nomenclature.

No. of elements	Mesh name	Time taken to complete simulation
64043	M1	36 min 3 seconds
117375	M2	41 min 57 seconds
304542	M3	3 hours 31 minutes 34 seconds
1024680	M4	8 hours 56 minutes 21 seconds

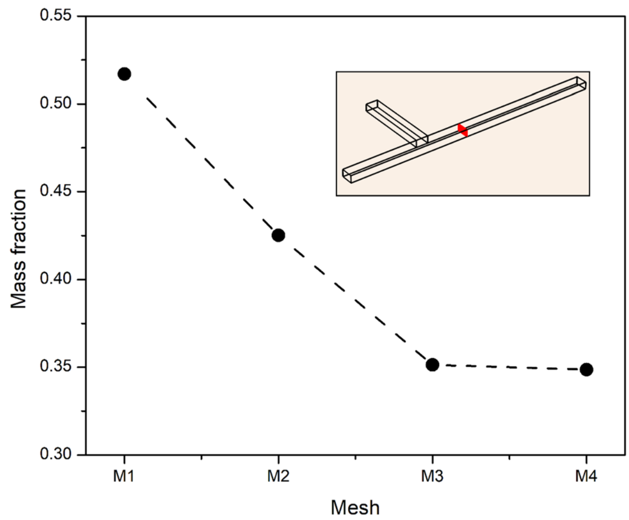

Figure 2. Mesh independence study. The plane at which the averaged mass fraction is taken shown in red color.

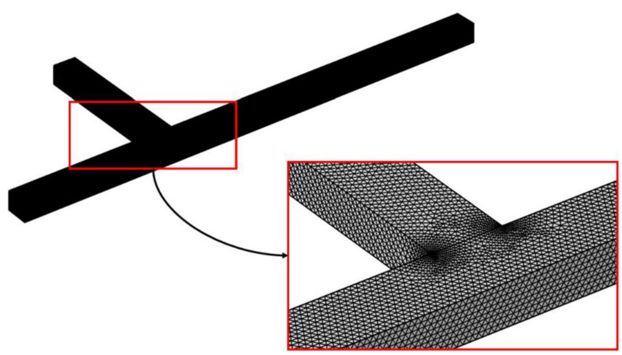

Figure 3. Mesh configuration M3 having tetrahedral mesh elements.

is the apparent viscosity of the non-Newtonian liquid which is governed by power law defined as follows-

$$\mu_{app} = k(\dot{\gamma})^{n-1} = m\left(\frac{\dot{\gamma}}{\dot{\gamma}_{ref}}\right)^{n-1} \quad (3)$$

where k is the flow consistency index, $\dot{\gamma}$ is the characteristic strain-rate, n is the flow behavior index, m is the modified flow consistency index with value taken to be the viscosity of the base fluid i.e. $m = 10^{-3}$ Pa-s, and $\dot{\gamma}_{ref}$ is the reference strain-rate which is taken as 1 s^{-1}.

The characteristic strain-rate $\dot{\gamma}$ is given as follows:

$$\dot{\gamma} = \sqrt{2\bar{\bar{S}} : \bar{\bar{S}}} \quad (4)$$

and $\bar{\bar{S}}$ is the strain-rate tensor, defined as follows:

$$\bar{\bar{S}} = \frac{1}{2}\left(\left(\nabla\vec{V}\right) + \left(\nabla\vec{V}\right)^{T}\right) \quad (5)$$

Species transport equation

$$\frac{\partial c}{\partial t} + (\mathbf{u}\cdot\nabla)c = D\,\nabla^2 c \quad (6)$$

Here, c is the concentration and D is the diffusion coefficient. As we intend to study the effect of time varying input on mixing of two liquids, both advective and diffusive component becomes important.

To model the pulsatile inlet velocity conditions at both the inlets, a sinusoidal equation is used given as [22] :

$$U = U_s + U_m \sin(2\pi f t + \varphi) \quad (7)$$

The steady-state velocity (U_s) is 1 mm/s and the maximum velocity, (U_m) is taken as 7.5 mm/s.

The boundary conditions associated with the aforementioned governing equations are as follows:

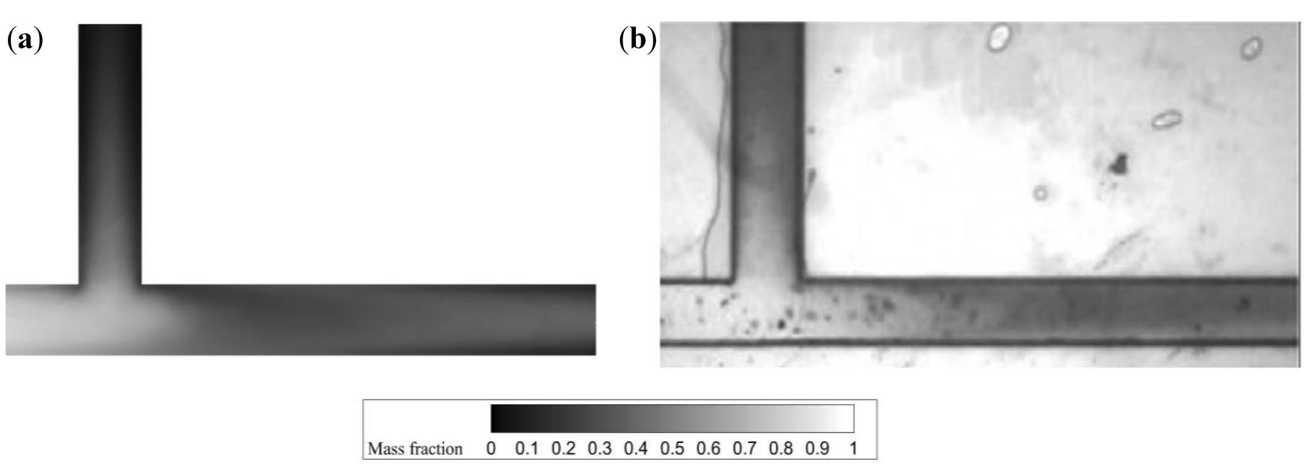

Figure 4. Validation with (**a**) Current Simulation and (**b**) Glasgow and Aubry [2].

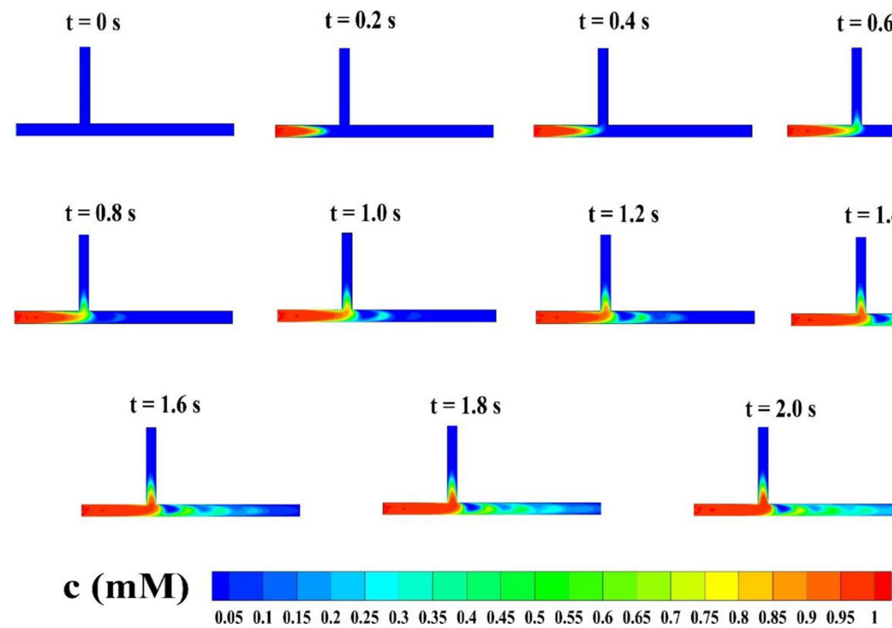

Figure 5. Evolution of pulsing in first 10 cycles. Mixing in channel starts from 10th cycle i.e. from t = 1.8 s.

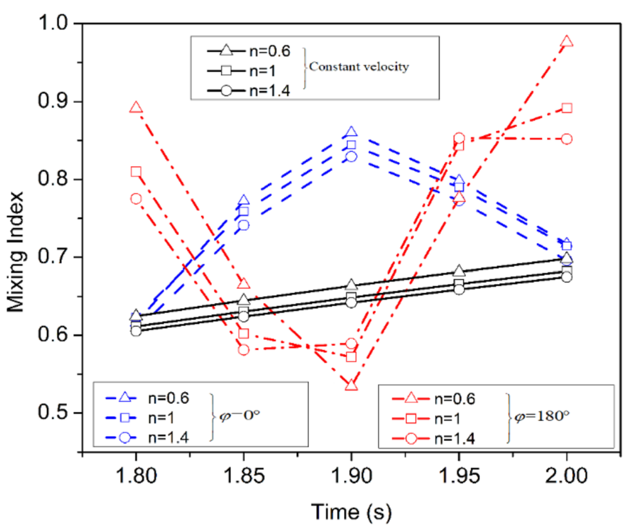

Figure 6. Variation of mixing index as a function of time for different inlet conditions.

- At walls, no slip and no flux boundary condition
- At inlet A-
  - $U = U_s + U_m \sin(2\pi f t)$.
  - $c = 0$ mM.
- At inlet B-
  - $U = U_s + U_m \sin(2\pi f t + \varphi)$.
  - $c = 1$ mM.
- At Outlet
  - $P = 1$ atm

Here we have considered, fluid A entering from inlet A and fluid B entering from inlet B. The properties of fluid A and fluid B are identical with density ρ = 1000 kg/m^3 and the diffusivity, D = 10^{-10} m^2/s. The outlet is assumed to be open to atmosphere and thus, a constant pressure of 1 atm is applied at the outlet. For studying the mixing characteristic of the liquids, we have considered concentration, "c" which is 0 mM for fluid A and 1 mM for fluid B. In the case of perfect mixing, the value of c is 0.5 mM which is denoted by c_∞ for no mixing c is 0 mM which is denoted by c_0. The non-Newtonian behavior is modeled using power law viz Eq. (3). The modified flow consistency index (m) is assumed to be 0.001 Pa.s. The flow behavior index (n) is assumed to be 0.6, 1 and, 1.4 which represents shear thinning ($n < 1$), Newtonian ($n = 1$) and shear thickening ($n > 1$) behavior respectively.

To show the efficiency of micro-mixer we calculated the Mixing Index (MI) at the outlet of the micro-mixer. The expression for the MI can be defined as [22]:

$$\mathrm{MI} = 1 - \frac{\int_s |c - c_\infty| ds}{\int_s |c_0 - c_\infty| ds} \quad (8)$$

where we have considered concentration, "c" which is 0 mM for fluid A and 1 mM for fluid B. In the case of perfect mixing, the value of c is 0.5 mM which is denoted by c_∞ for no mixing c is 0 mM which is denoted by c_0.

Where, MI represents,

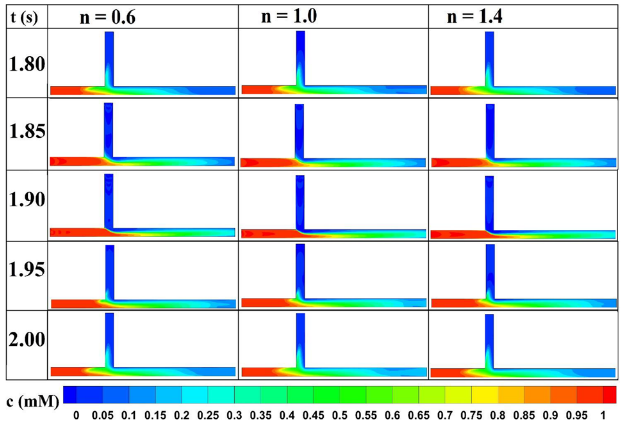

Figure 7. Variation in concentration at the centre plane for φ = 0°.

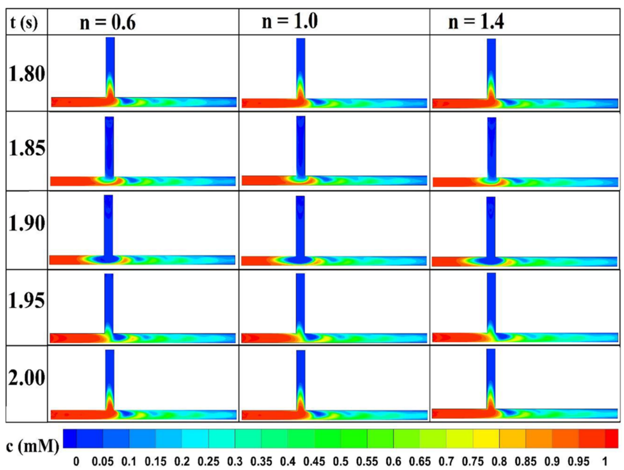

Figure 8. Variation in concentration at the centre plane for φ = 180°.

$$\mathrm{MI} = \begin{cases} 1, & \text{Perfect mixing} \\ 0 < \mathrm{MI} < 1, & \text{Mixed fluid} \\ 0, & \text{No mixing} \end{cases} \quad (9)$$

2.3 *Validation and mesh independence study*

Mesh independence study is performed with varying mesh sizes or the number of elements mentioned in Table 1. It is observed from figure 2 that after mesh M3, the variation in mass fraction of the fluid is negligible. The computational time however, increases significantly for the M4 mesh. Therefore, we have opted for M3 for further study (figure 3).

The numerical model is validated with the experiment data of Glasgow and Aubry [2]. They studied the effect of pulsatile velocity at inlet on mixing of two Newtonian liquids with identical density and diffusivity in a microchannel. The fluid used in the literature [2] is water and at the inlet, the flow velocity is assumed to be pulsating in nature where the velocity is defined as $1.0 + 7.5\,sin(5 \times 2\pi t)$ mm/s at the inline inlet and $1.0 + 7.5\,sin(5 \times 2\pi t + \varphi)$ mm/s at perpendicular inlet. The outlet is open to atmosphere.

To validate our model, we used power law model with m = 0.001 Pa.s and n = 1. A comparison of the mass fraction of a fluid after the pulsing is established in the channel (i.e. after 10th cycle [2]) is shown in figure 4 and the numerical data is in good agreement. Also, the time-averaged mixing index obtained from our simulations is 0.57 which is within 2% of the value reported by Glasgow and Aubry [2].

3. Results and discussion

All the simulations are performed in FEM based commercial software COMSOL Multiphysics. In the present study, the effect of pulsed input, phase angle (0° and 180°), and pulsing frequency (5 Hz to 20 Hz) on the mixing characteristics of non-Newtonian liquids are discussed. All the readings are taken when the pulsing is fully established i.e., at least after 10 periods [2]. The readings are taken at a location 0.75 mm after confluence. Figure 5 shows the evolution of two fluids in the first 10 cycles.

3.1 *Effect of pulsed input*

We begin by comparing the mixing of various non-Newtonian fluids with different flow behavior index, n ranging from 0.6 to 1.4, in a T shape microchannel with and without pulsed input. For the case of pulsed flow, the results have been taken when pulsed flow is fully established (for the present study from 1.8 to 2 s) as shown in figure 5. Figure 6 shows that the mixing index for shear thinning liquid is higher and for shear thickening liquid is lower after a complete cycle as compared to the Newtonian fluid regardless of input condition (pulsed i.e. for φ = 0° or constant velocity input). This is because for the shear thinning case, with the decrease in flow behavior index, the apparent viscosity decreases which increase the flow mobility and consequently mixing enhances. Whereas, for the shear thickening case, with an increase in flow behavior index, the apparent viscosity increases and thereby reduces the mixing. It can be noted that, in the case of constant input velocity, mixing enhances linearly with time (depicted by black curve in figure 6). However, for the case of pulsed input condition, mixing enhances, and attains maximum mixing at half cycle; and beyond that, it decreases with time (depicted by blue curves in figure 6). This is because fluids from both the inlets are being pushed in the channel simultaneously in the first half of the pulse i.e., from 1.8 to 1.9 s while in the second half of the cycle (1.9–2

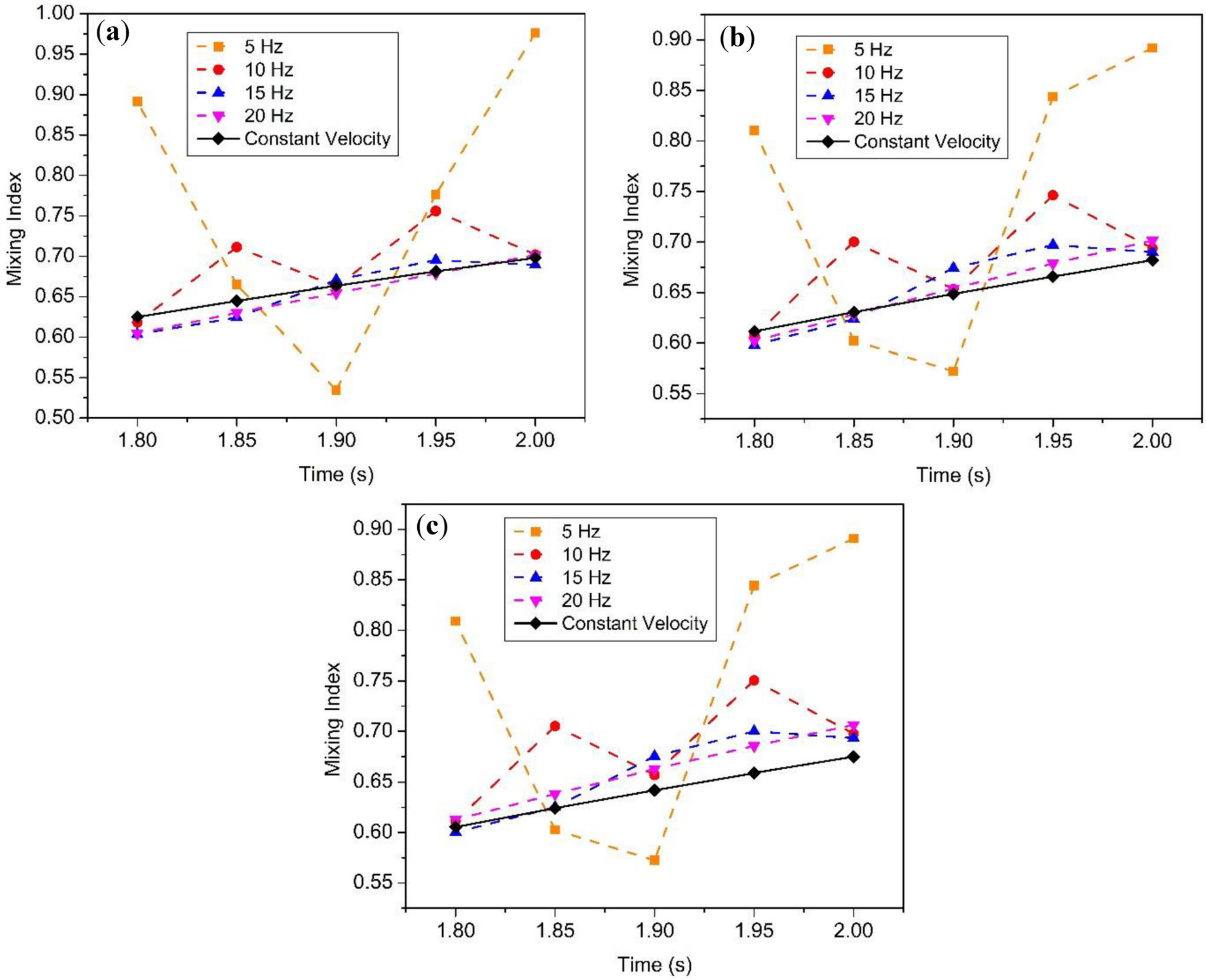

Figure 9. Effect of frequency on mixing index of (**a**) shear thinning fluid (n = 0.6), (**b**) Newtonian fluid (n = 1) and (**c**) shear thickening fluid (n = 1.4).

s) fluids are being pulled back from the channel (see figure 7). For the case of constant input flow, the mixing index is 69.8%, 68.2%, and 67.5% for flow behavior index, n = 0.6, 1 and 1.4 respectively whereas for the case of pulsed flow, the mixing index is 71.7%, 71.4% and 69.5% for flow behavior index, n = 0.6, 1 and 1.4 respectively, after full cycle, (t = 2 s). However, for the case of pulsed input, the maximum mixing index is achieved at half cycle with 86%, 84.4%, and 82.9% for flow behavior index, n = 0.6, 1 and 1.4 respectively.

3.2 *Effect of phase angle*

In this section, the effect of phase angle on the mixing index is studied for all the fluids mentioned above. We compare the input condition of 180° phase difference with the standard pulsing case (φ = 0°) considering the frequency to be 5 Hz. Figure 6 reveals an opposite trend for φ = 0° and φ = 180°. For φ = 180°, the mixing index reduces with time up to half a cycle and increases beyond that regardless of fluid rheology. This is because for the first half cycle (1.8–1.9 s), as time increases, the fluid is being pushed in from inlet A and pulled out from other inlet B; this results in filling in the channel with only a single fluid during first half cycle as shown in figure 8. For the second half cycle (1.9–2 s), the fluid from the inlet A is pulled out and from inlet B is being pushed in. This alternating motion creates a recirculating flow at the junction which enhances mixing (see figure 7). It can be noted from figure 6 that, for the case of φ = 180°, the maximum mixing is achieved after the full cycle with the mixing index, of 97.6%, 89.1% and 85.2% for n = 0.6, n = 1 and n = 1.4, respectively.

3.3 *Effect of frequency of pulsation*

As discussed in the aforementioned section, the highest mixing is achieved for pulsed input condition of 180° phase difference. Therefore, considering the same phase difference, we vary the frequency of pulsation ranging from 5 to 20 Hz and investigate its impact on the mixing of different fluid rheology. From figure 9, it can be seen that with increasing frequency, the mixing index decreases regardless of fluid rheology. This is due to the fact that with increasing frequency, the full cycle time decreases because of an increase in the number of cycles for a fixed range of time (1.8–2.0 s) and thereby, fluids do not get enough time to diffuse. As a consequence, mixing decreases. It can be also observed that for lower frequency, the mixing index decreases in the first half of the cycle and increases in the second half. This is because a phase difference of 180° physically implies the fluids are being pushed in the channel in an alternating manner. This implies that in the first half of the pulse cycle, there is only one fluid present in the channel. The mixing begins in the next half when the second fluid gets pushed in and consequently, a rise in mixing index is observed. The variation in pattern of the mixing index, with time, is observed to change with increasing frequency. This is attributed to an increase in the number of cycles for a fixed range of time. It is interesting to note that the mixing index reduces significantly from 5 to 10 Hz and the variations are minor beyond 10 Hz.

4. Conclusions

We have numerically investigated the fluid mixing in a T-shaped channel geometry at micro scale with perpendicular inlets for constant velocity, standard pulsing case ($\varphi = 0°$), and pulsing inlet with 180° phase difference for various non-Newtonian fluids. We demonstrate that the mixing of fluid increases for shear-thinning liquids. Also, it is evident that the standard pulsed flow improves the mixing marginally as compared to the constant velocity for the full cycle. However, for the case of the half cycle, the standard pulsed flow gives a maximum mixing index which is 86%, 84.4% and 82.9% for $n = 0.6$, $n = 1$, and $n = 1.4$ respectively. Next, we achieve the highest mixing by increasing the phase difference of pulsed input to 180° considering a frequency of 5 Hz with the mixing index of 97.6% after the full cycle which occurs for shear-thinning fluid ($n = 0.6$). Lastly, we investigate the effect of frequency on the mixing index and note that with an increase in frequency, the mixing index reduces. Finally, it can be concluded that, for enhancing mixing in non-Newtonian fluids obeying the power law model, the pulsatile inlet condition along with a lower frequency is an effective technique and the best mixing can be achieved with a phase difference of 180°. The present study will be helpful in designing micromixers for better and more effective fluid mixing in a small time and length span of the channel.

List of symbols

c	Concentration, mM
D	Diffusion coefficient, m^2/s
f	Frequency, Hz
$\mathbf{I}$	Identity matrix
k	Flow consistency index, $Pa.s^n$
m	Modified flow consistency index, Pa.s
MI	Mixing index
n	Flow behavior index
p	Pressure, Pa
t	Time, s
U	Inlet velocity function, m/s
U_m	Maximum velocity, m/s
U_s	Steady state velocity, m/s
$\mathbf{u}$	Velocity vector, m/s
Γ	Rate of strain, 1/s
μ_{app}	Apparent viscosity, Pa. s
φ	Phase angle, °
ρ	Density of fluid, kg/m^3

Greek symbols

Γ	Rate of strain, 1/s
μ_{app}	Apparent viscosity, Pa. s
φ	Phase angle, °
ρ	Density of fluid, kg/m^3

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